CompassCDS
Enhanced Chromatogram Report
Plug-in User Guide

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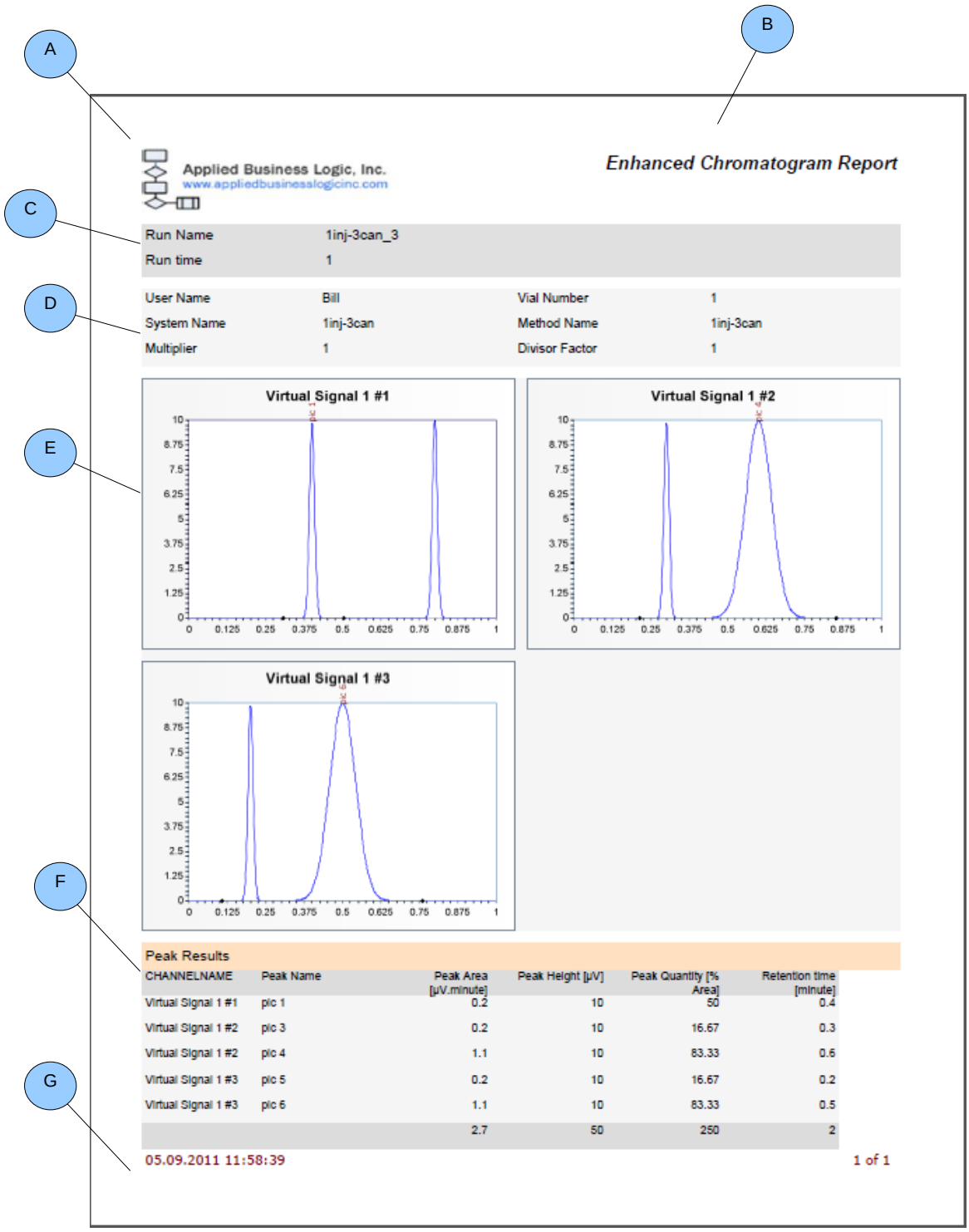
Introduction

The Enhanced Chromatogram Reporter produces a customizable graphical / tabular view of all data for a given run. The report displays a chromatogram for all channels (1 to 4), along with a table of results for each peak. The report is configured as a CompassCDS post-run plug-in but can also be run in Direct Mode via the toolbar menu Plug-ins option. The process renders the report in the industry standard PDF format which is read using Adobe Reader.

This document describes the advanced features and configuration of this report.

The Enhanced Chromatogram Report at a Glance


A
B
C
D
E
F
G
Applied Business Logic, Inc.
www.appliedbusinesslogicinc.com
Enhanced Chromatogram Report
Run Name 1inj-3can_3
Run time 1
User Name Bill
Vial Number 1
System Name 1inj-3can
Method Name 1inj-3can
Multiplier 1
Divisor Factor 1
Virtual Signal 1 #1
Virtual Signal 1 #2
Virtual Signal 1 #3
Peak Results
CHANNELNAME Peak Name Peak Area [µV.minute] Peak Height [µV] Peak Quantity [% Area] Retention time [minute]
Virtual Signal 1 #1 pic 1 0.2 10 50 0.4
Virtual Signal 1 #2 pic 3 0.2 10 16.67 0.3
Virtual Signal 1 #2 pic 4 1.1 10 83.33 0.6
Virtual Signal 1 #3 pic 5 0.2 10 16.67 0.2
Virtual Signal 1 #3 pic 6 1.1 10 83.33 0.5
2.7 50 250 2
05.09.2011 11:58:39
1 of 1

A. Custom header graphics are interchangeable and users can insert a company logo onto the report. This is done by simply re-naming the “logo.jpg” that is located in the C:\Program Files\Scion\Enhanced Chromatogram Report\ folder and replacing it with the desired logo named ‘logo.jpg’. The logo will be displayed in the upper-right corner of the report (300X100 px graphic).

B. Report Name can be configured via configuration dialog.

C. Page Header appears at the top of each page and can be configured using any CompassCDS Global variables.

D. Report header appears at the top of the first page and can be configured using any CompassCDS Global variables.

E. Graphical chromatograms shown for up to four detector channels.

F. The Peak Results table is displayed below the chromatogram. The table can be separated by channel, or all of the results combined into a single table. Group Results are supported in the same way. Group table(s) appear after Peak Result tables. Peak and Group table columns are configured via the configuration dialog.

G. The report footer shows time/date (in localized format), and page number.

Software Prerequisites

- The plug-in requires .NET Framework 3.5. The installer will prompt the user to install if it has not been installed. This application can be found in the Tools folder on the CompassCDS DVD or downloaded from https://www.microsoft.com/en-us/download/details.aspx?id=21
- Microsoft Report Viewer Redistributable 2008: https://www.microsoft.com/en-us/download/details.aspx?id=6576
- Adobe Reader, used to read PDF files. This application can be found on the CompassCDS DVD or downloaded and installed from: https://get.adobe.com/de/reader/?promoid=BUIGO
- CompassCDS Version 4.0 or higher.

Installing the Enhanced Chromatogram Report Plug-in

1. Using Windows Add/Remove Programs, uninstall any previously installed version of the Enhanced Chromatogram Report Plug-in.

2. Run the attached Setup.exe file and follow the prompts to complete the install.

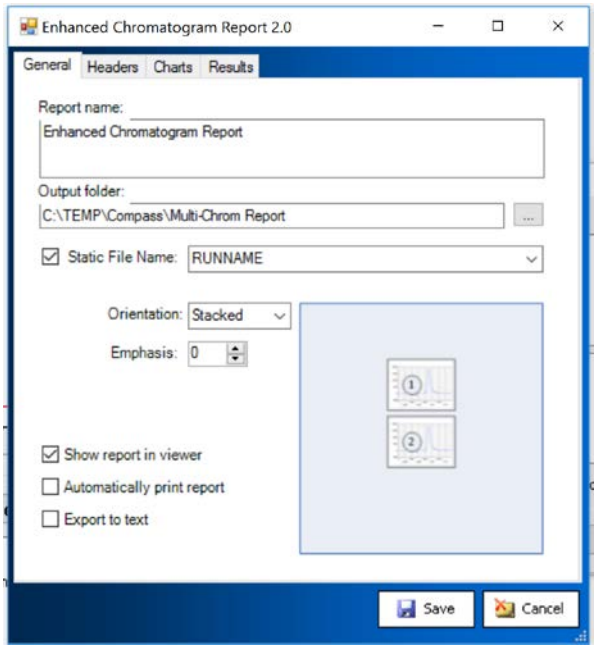
Configuring the Enhanced Chromatogram Report Plug-in

1. The CompassCDS Enhanced Chromatogram Report is configured as a post-run plug-in within the CompassCDS method. Click the post-processing section of the method, then click Add and follow the steps to add the plug-in.

NOTE: If the plug-in does not appear in the CompassCDS list for post-run plug-ins, double click the included MultiChannelChromatogramReport.reg file to manually register the plug-in. Restart CompassCDS.

2. Once the plug-in has been added to the method, it must be configured. Click the Configure button on the CompassCDS dialog.

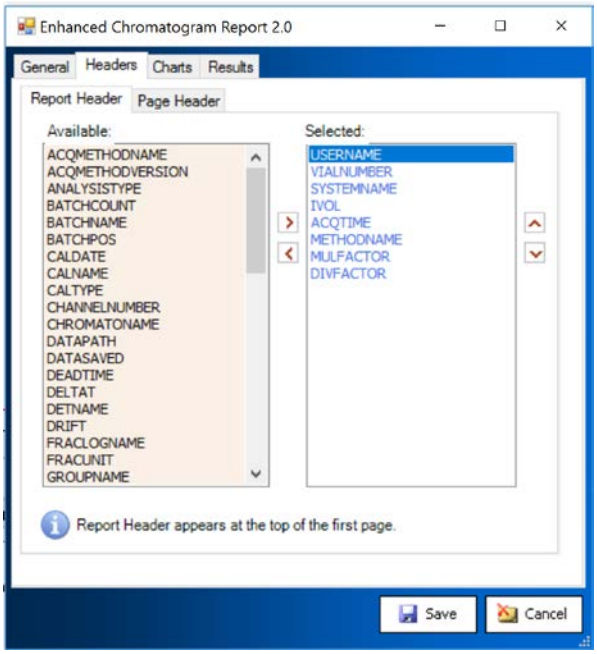
Configuring the General Settings



1. Specify the Report Name to appear in the Report Header
2. Select the output folder where all reports will be written.
3. Select the option to use a static file name based on any CompassCDS Global Variable. If left unchecked, the program creates a random (unique) file name.
4. Control the orientation of the chromatograms appearing on the report (Stacked or Standard).
5. Set the Emphasis on a particular channel to make this chromatogram larger than the rest.
6. Check to show the report in the Adobe Reader viewer after the PDF file has been created.
7. Check to enable silent printing of the report to the default printer without showing the chromatogram in the viewer.

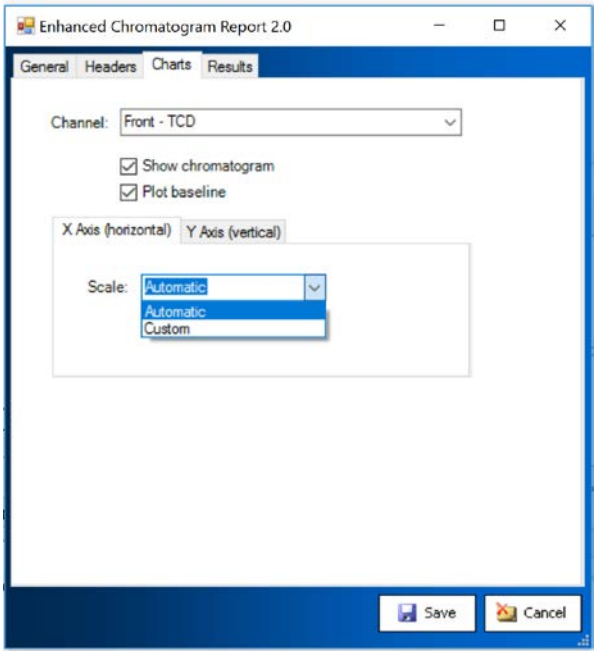
Configuring the Headers

The CompassCDS Enhanced Chromatogram Report has two header sections; Report Header and Page Header. Each is configured separately.



1. The Report Header is displayed only at the top of the first page.
2. The Page Header is displayed at the top of each page.
3. Users may configure each header section by selecting from a list of CompassCDS variables that can include custom variables.

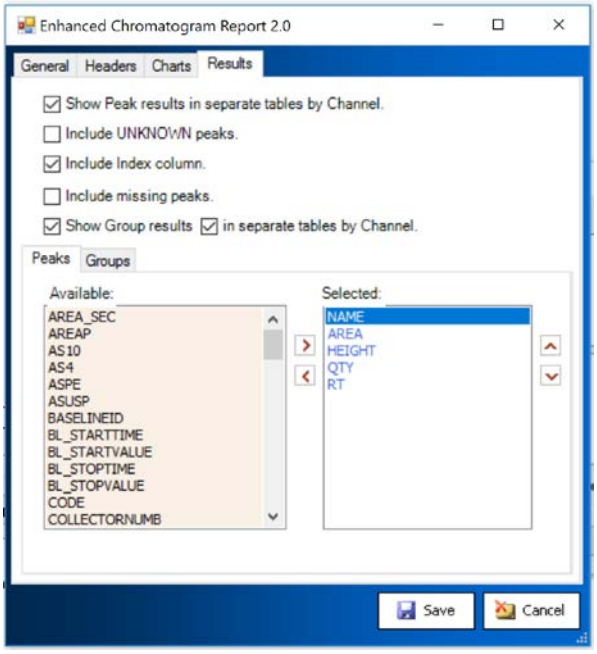
Configuring Charts



Select the channel from the Channel dropdown. For each channel, the following changes can be made:

- Click Show chromatogram to have the selected channel appear on the report.
- Select Plot Baseline to have the baseline plotted in the graph.
- Select Include UNKNOWN peaks to include the UNKNOWN summary row in the tabular output.
- The scale for both X and Y axis can be configured independently for each channel. Selecting Automatic (default) allows the charting program render a best-fit scale. Choosing Custom allows the user to specify a From and To value for a given axis.

Configuring Results Display



1. The report can display PEAK results in separate tables (per channel), or combine all results into a single table.
2. The report can include or exclude UNKNOWN peaks.
3. Include/exclude the index (row count) column in the tabular output.
4. Users can choose to include missing peaks, where peaks specified in the method were not detected in the run. Results values for these peaks will be zero.
5. The report can show GROUP results in separate tables (per channel), or combine all GROUP results into a single table.
6. Users can select tabular report columns for PEAKS by selecting from available CompassCDS variables/custom variables at the peak level.
7. Users can select tabular report columns for GROUPS by picking from available CompassCDS variables/custom variables at the group level.

Configuration Defaults

When the CompassCDS Enhanced Chromatogram Report is first configured in the post-run section of the method (or data file), the defaults for all settings are managed via the ecr.config file. Special care must be taken when editing this file. Examples below:

- Default the report name:
  <Setting Name="DEFAULT_REPORTNAME" Value="Enhanced Chromatogram Report" />
- Default columns for peak results table (comma-separated list):
  <Setting Name="DEFAULT_PEAKVARIABLES" Value="NAME,AREA,HEIGHT,QTY,RT" />

Running the CompassCDS Enhanced Chromatogram Report Plug-in

Post Run: Once configured, the CompassCDS Enhanced Chromatogram Report plug-in runs automatically after each run. During this process, raw data is gathered from CompassCDS via the API and then transformed into each chart. The results table is also built using CompassCDS API calls. The report is rendered into .PDF format and can be read using the Adobe Reader application. Depending on the size of the data file, this process can take as long as 30 seconds to complete.

Direct Mode: The CompassCDS Enhanced Chromatogram Report plug-in can also be launched from the main CompassCDS toolbar. The “Plug-in menu item” on the toolbar launches the report. Note: a CompassCDS Chromatogram method file MUST be loaded into the Data view for this to work.

Logging

During report execution, messages are written to log.txt file found in the logged-in users’ Application Data folder (C:\Documents and Settings\User1\Application Data). These include tracing/status messages along with error messages.